Anthony Scemama

List of Publications by Year
in descending order

23 papers	824 citations	567281 15 h-index	642732 23 g-index
23 all docs	23 docs citations	23 times ranked	583 citing authors

#	Article	IF	Citations
1	Quantum Package 2.0: An Open-Source Determinant-Driven Suite of Programs. Journal of Chemical Theory and Computation, 2019, 15, 3591-3609.	5.3	108
2	Hybrid stochastic-deterministic calculation of the second-order perturbative contribution of multireference perturbation theory. Journal of Chemical Physics, 2017, 147, 034101.	3.0	106
3	Selected configuration interaction dressed by perturbation. Journal of Chemical Physics, 2018, 149, 064103.	3.0	92
4	<scp>QUESTDB</scp>: A database of highly accurate excitation energies for the electronic structure community. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2021, 11, e1517.	14.6	84
5	Excitation energies from diffusion Monte Carlo using selected configuration interaction nodes. Journal of Chemical Physics, 2018, 149, 034108.	3.0	50
6	Communication: Toward an improved control of the fixed-node error in quantum Monte Carlo: The case of the water molecule. Journal of Chemical Physics, 2016, 144, 151103.	3.0	48
7	Deterministic Construction of Nodal Surfaces within Quantum Monte Carlo: The Case of FeS. Journal of Chemical Theory and Computation, 2018, 14, 1395-1402.	5.3	48
8	Excited States with Selected Configuration Interaction-Quantum Monte Carlo: Chemically Accurate Excitation Energies and Geometries. Journal of Chemical Theory and Computation, 2019, 15, 4896-4906.	5.3	34
9	Chemically accurate excitation energies with small basis sets. Journal of Chemical Physics, 2019, 151, 144118.	3.0	30
10	Excited States from State-Specific Orbital-Optimized Pair Coupled Cluster. Journal of Chemical Theory and Computation, 2021, 17, 4756-4768.	5.3	29
11	Quantum Monte Carlo for large chemical systems: Implementing efficient strategies for petascale platforms and beyond. Journal of Computational Chemistry, 2013, 34, 938-951.	3.3	28
12	The performance of CIPSI on the ground state electronic energy of benzene. Journal of Chemical Physics, 2020, 153, 176101.	3.0	26
13	A Jeziorski-Monkhorst fully uncontracted multi-reference perturbative treatment. I. Principles, second-order versions, and tests on ground state potential energy curves. Journal of Chemical Physics, 2017, 146, 224108.	3.0	25
14	Tailoring CIPSI Expansions for QMC Calculations of Electronic Excitations: The Case Study of Thiophene. Journal of Chemical Theory and Computation, 2021, 17, 3426-3434.	5.3	17
15	A basis-set error correction based on density-functional theory for strongly correlated molecular systems. Journal of Chemical Physics, 2020, 152, 174104.	3.0	16
16	Toward a systematic improvement of the fixed-node approximation in diffusion Monte Carlo for solidsâ€"A case study in diamond. Journal of Chemical Physics, 2020, 153, 184111.	3.0	16
17	A simple approach to the state-specific MR-CC using the intermediate Hamiltonian formalism. Journal of Chemical Physics, 2016, 144, 064101.	3.0	14
18	Accurate full configuration interaction correlation energy estimates for five- and six-membered rings. Journal of Chemical Physics, 2021, 155, 134104.	3.0	14

#	Article	IF	Citations
19	Taming the fixed-node error in diffusion Monte Carlo via range separation. Journal of Chemical Physics, 2020, 153, 174107.	3.0	11
20	Reference Energies for Cyclobutadiene: Automerization and Excited States. Journal of Physical Chemistry A, 2022, 126, 4664-4679.	2.5	11
21	Alternative definition of excitation amplitudes in multi-reference state-specific coupled cluster. Journal of Chemical Physics, 2017, 146, 154107.	3.0	8
22	Reference Excitation Energies of Increasingly Large Molecules: A QMC Study of Cyanine Dyes. Journal of Chemical Theory and Computation, 2022, 18, 1089-1095.	5.3	7
23	The effect of uncertainty on building blocks in molecules. Journal of Chemical Physics, 2022, 156, .	3.0	2